Mecânica Quântica

Oscilador Harmônico

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Prof. Hans Dessens

Oscilador Harmônico

Hamiltoniano

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2}$$

Logo, temos a equação

$$\hat{H}\psi = E\psi$$

$$\left(\frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}}{2} \right) \psi = E\psi$$

Podemos definir os operadores

$$\hat{a} = \frac{1}{\sqrt{2\hbar m\omega}} \left(m\omega \hat{x} + i\hat{p} \right)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}} \left(m\omega \hat{x} - i\hat{p} \right)$$

De modo que

$$\hat{a}^\dagger \hat{a} = \frac{1}{2\hbar m\omega} \left(m\omega \hat{x} - i\hat{p} \right)\left(m\omega \hat{x} + ip \right)$$

$$= \frac{1}{2\hbar m\omega} \left(m^2\omega^2 \hat{x}^2 + im\omega \hat{x}\hat{p} - im\omega \hat{p}\hat{x} + \hat{p}^2 \right)$$

$$\hat{a}^\dagger\hat{a} = \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + m^2\omega^2\hat{x}^2 + im\omega\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)\right)$$

$$\hat{a}^\dagger\hat{a} = \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2} - \frac{\hbar\omega}{2}\right)$$

$$\hat{a}^\dagger\hat{a} = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}$$

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \qquad [\hat{a}, \hat{a}^\dagger] = 1$$

Portanto,

$$\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)\psi = E\psi$$

Operador criação $\hat{a}^\dagger$

$$\hat{H}\left(\hat{a}^\dagger\psi\right) = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}^\dagger\psi$$

$$= \hbar\omega\left(\hat{a}^\dagger\hat{a}\hat{a}^\dagger + \frac{\hat{a}^\dagger}{2}\right)\psi$$

$$= \hbar\omega\hat{a}^\dagger\left(\hat{a}\hat{a}^\dagger + \frac{1}{2}\right)\psi \qquad \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$$
$$\hat{a}\hat{a}^\dagger = 1 + \hat{a}^\dagger\hat{a}$$

$$= \hbar\omega a^\dagger\left(a^\dagger a + 1 + \frac{1}{2}\right)\psi$$

$$\hat{H}(\hat{a}\psi) = \hat{a}^{\dagger}\left(\hbar\omega\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right) + \hbar\omega\right)\psi$$

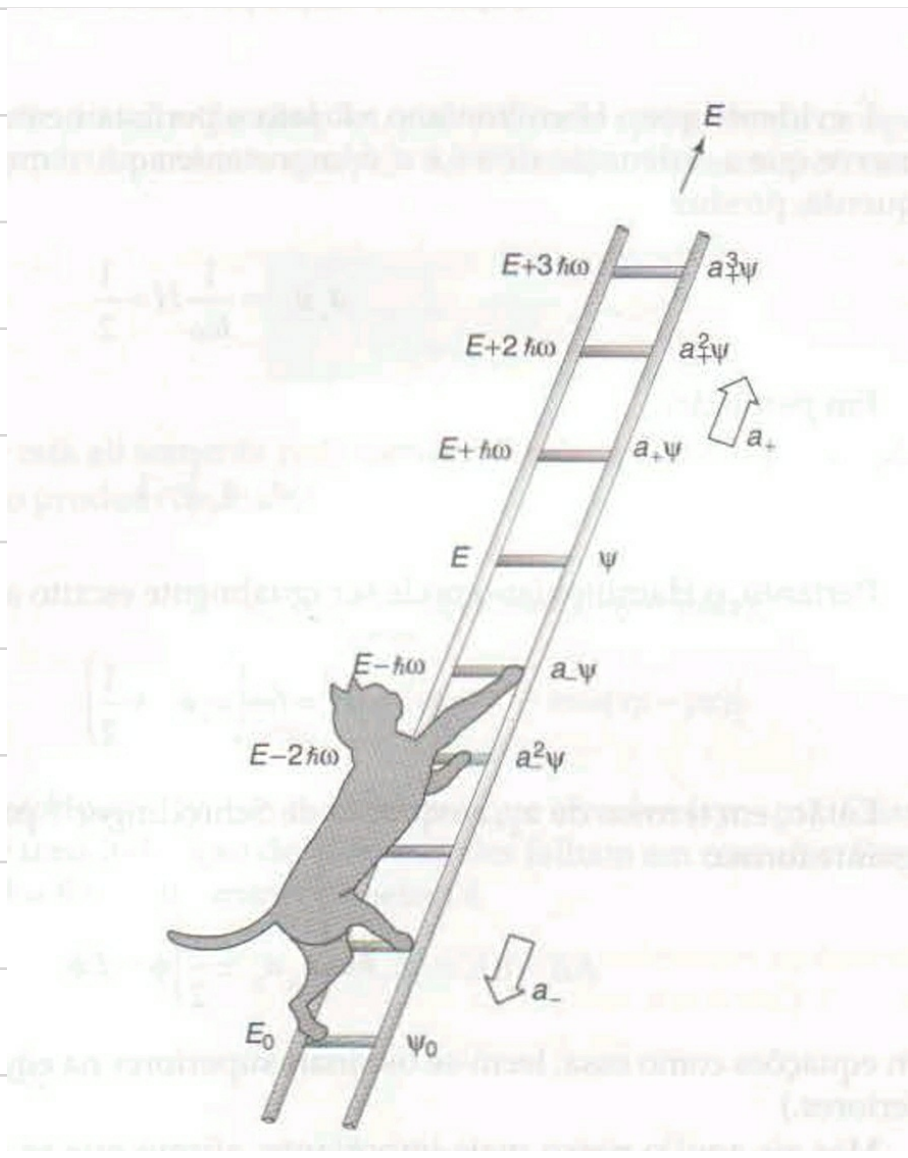
$$\hat{H}(\hat{a}^{\dagger}\psi) = \hat{a}^{\dagger}(\hat{H} + \hbar\omega)\psi$$

$$\hat{H}(\hat{a}^{\dagger}\psi) = \hat{a}^{\dagger}(E + \hbar\omega)\psi$$

$$\hat{H}(\hat{a}^{\dagger}\psi) = (E + \hbar\omega)(\hat{a}^{\dagger}\psi)$$

↳ O operador $\hat{a}^{\dagger}$ produz novas soluções com energias maiores.

↳ De maneira análoga, $\hat{a}$ produz soluções com energias menores (operador destruição).



$$\psi_n \rightarrow E_n$$
$$\hat{a}^{\dagger}\psi_n \rightarrow \psi_{n+1} \rightarrow E_{n+1}$$
$$\hat{a} \rightarrow \psi_{n-1} \rightarrow E_{n-1}$$

Estado fundamental

$$\hat{a}\psi_0 = 0$$

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega\hat{x} + i\hat{p}\right)\psi_0 = 0$$

$$\left(m\omega x + i\left(-i\hbar\frac{\partial}{\partial x}\right)\right)\psi_0 = 0$$

$$m\omega x\psi_0 + \hbar\frac{d\psi_0}{dx} = 0$$

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar} x\, \psi_0$$

$$\frac{d\psi_0}{\psi_0} = -\frac{m\omega}{\hbar} x\, dx$$

$$\ln \psi_0 = -\frac{m\omega x^2}{2}$$

$$\psi_0 = A e^{-\frac{m\omega x^2}{2}}$$

$$\int |\psi_0|^2 dx = 1$$

$$|A|^2 \int e^{-\frac{m\omega x^2}{2}} dx = 1$$

$$|A|^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1$$

$$A^2 = \sqrt{\frac{m\omega}{\pi\hbar}}$$

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

Portanto,

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2}}$$

A energia do estado fundamental é

$$\hat{H}\psi_0 = E_0\psi_0$$

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\psi_0 = E_0\psi_0$$

$$\frac{\hbar\omega}{2}\psi_0 = E_0\psi_0$$

$$E_0 = \frac{\hbar\omega}{2}$$

Assim, podemos escrever

$$\psi_n(x) = A_n\left(\hat{a}^\dagger\right)^n\psi_0(x) \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Podemos definir o operador número, tal que

$$\hat{H}\psi_n = E_n\psi_n$$

$$\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\psi_n = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n$$

$$\hat{a}^\dagger\hat{a}\psi_n = n\psi_n \qquad \hat{N} = \hat{a}^\dagger\hat{a}$$

$$\hat{N}\psi_n = n\psi_n$$

Constantes de normalização

$$\hat{a}^\dagger \psi_n = c_n \psi_{n+1} \qquad \hat{a}\,\psi_n = d_n \psi_{n-1}$$

Note que

$$\int \varphi^* \hat{a}^\dagger \chi \, dx = \frac{1}{\sqrt{2\hbar m\omega}} \int \varphi^* \left(m\omega \hat{x} + i\hat{p} \right) \chi \, dx$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int \varphi^* \left(m\omega x + i\left(-i\hbar \frac{d}{dt} \right) \right) \chi \, dx$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \left| \int \varphi^* m\omega x \, \chi \, dx + \hbar \int \varphi^* \frac{d}{dt} \psi \, dx \right|$$

$$\int \varphi^* \frac{d}{dx} \chi = \varphi^* \psi - \int \psi \frac{d\varphi^*}{dx} dx = -\int \psi \left(\frac{d\varphi}{dx} \right)^* dx$$

$$\int \varphi^* \hat{a}^\dagger \chi \, dx = \frac{1}{\sqrt{2\hbar m\omega}} \left| \int \varphi^* m\omega x - \hbar \int \left(\frac{d\varphi}{dx} \right)^* \psi \, dx \right|$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int \left| \left[m\omega x - \hbar \frac{d}{dx} \right] \varphi \right|^* \psi \, dx$$

$$\int \varphi^* \hat{a} \chi \, dx = \int \left(\hat{a}^\dagger \varphi \right)^* \chi \, dx$$

Dessa forma,

$$\int (\hat{a}\psi_n)^* (\hat{a}\psi_n) = \int (\hat{a}^\dagger \hat{a}\psi_n)^* \psi_n \, dx$$

$$\int d_n^* \psi_{n-1}^* \, d_n \psi_{n-1} \, dx = n \int \psi_n^* \psi_n \, dx$$

$$|d_n|^2 \int |\psi_{n+1}|^2 dx = n \int |\psi_n|^2 dx$$

$$d_n = \sqrt{n}$$

Além disso,

$$\int (\hat{a}^\dagger \psi_n)^* (\hat{a}^\dagger \psi_n) dx = \int (\hat{a}\hat{a}^\dagger \psi_n)^* \psi_n \, dx$$

$$\int c_n^* \psi_{n+1}^* \, c_n \psi_{n+1} \, dx = (n+1) \int \psi_n^* \psi_n \, dx$$

$$|c_n|^2 \int |\psi_{n+1}|^2 dx = (n+1) \int |\psi_n|^2 dx$$

$$c_n = \sqrt{n+1}$$

Portanto,

$$\hat{a}^\dagger \psi_n = \sqrt{n+1}\, \psi_{n+1} \qquad \hat{a}\psi_n = \sqrt{n}\, \psi_{n-1}$$

Exemplos

$$\psi_1 = a_+ \psi_0 \qquad \hat{a}^\dagger \psi_1 = \sqrt{2}\, \psi_2$$

$$\psi_2 = \frac{1}{\sqrt{2}} \hat{a}^\dagger \psi_1 = \frac{1}{\sqrt{2}} (\hat{a}^\dagger)^2 \psi_0$$

$$\psi_3 = \frac{1}{\sqrt{3}} \cdot \hat{a}^\dagger \psi_2 = \frac{1}{\sqrt{3 \cdot 2}} (\hat{a}^\dagger)^3 \psi_0$$

Generalizando,

$$\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0$$

Exemplo 2.5 : Valor esperado da energia potencial

$$\langle \hat{V} \rangle = \left\langle \frac{1}{2} m\omega \hat{x}^2 \right\rangle = \frac{1}{2} m\omega \langle \hat{x}^2 \rangle$$

$$\langle \hat{V} \rangle = \frac{1}{2} m\omega \int \psi_n^* \hat{x}^2 \psi_n \, dx$$

Porém,

$$\hat{a} = \frac{1}{\sqrt{2\hbar\omega m}} (m\omega \hat{x} + i\hat{p})$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2\hbar m\omega}} (m\omega \hat{x} - i\hat{p})$$

$$\hat{a} + \hat{a}^\dagger = \frac{2m\omega}{\sqrt{2\hbar m\omega}} \hat{x}$$

$$\hat{x} = \frac{\sqrt{2\hbar m\omega}}{2m\omega}\left(\hat{a} + \hat{a}^{\dagger}\right)$$

$$\boxed{\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^{\dagger}\right)}$$

$$\hat{a}^{\dagger} - \hat{a} = \frac{-2i\hat{p}}{\sqrt{2\hbar m\omega}}$$

$$\hat{p} = \frac{-\sqrt{2\hbar m\omega}}{2i}\left(\hat{a}^{\dagger} - \hat{a}\right)$$

$$\boxed{\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^{\dagger} + \hat{a}\right)}$$

$$\hat{x}^2 = \frac{\hbar}{2m\omega}\left(\hat{a} + \hat{a}^{\dagger}\right)\left(\hat{a} + \hat{a}^{\dagger}\right)$$

$$\hat{x}^2 = \frac{\hbar}{2m\omega}\left(\hat{a}^2 + \hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} + \left(\hat{a}^{\dagger}\right)^2\right)$$

$$\langle \hat{V} \rangle = \frac{1}{2}m\omega^2 \cdot \frac{\hbar}{2m\omega}\int \psi_n^* \left(\hat{a}^2 + \hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} + \left(\hat{a}^{\dagger}\right)^2\right)\psi_n dx$$

$$\langle \hat{V} \rangle = \frac{\hbar\omega}{4}\left[\int \psi_n^* \hat{a}^2 \psi_n dx + \int \psi_n^* \hat{a}\hat{a}^{\dagger}\psi_n dx + \int \psi_n^* \hat{a}^{\dagger}\hat{a}\,\psi_n dx + \int \psi_n^* \left(\hat{a}^{\dagger}\right)^2 \psi_n dx\right]$$

$$\langle \hat{v} \rangle = \frac{\hbar\omega}{4} \left| c_1 \int \psi_n^* \psi_{n-2}\, dx + (n+1) \int \psi_n^* \psi_n\, dx \right.$$

$$\left. + n \int \psi_n^* \psi_n\, dx + c_2 \int \psi_n^* \psi_{n+2}\, dx \right|$$

$$\langle \hat{v} \rangle = \frac{\hbar\omega}{4} \left(n+1+n \right)$$

$$\langle \hat{v} \rangle = \frac{\hbar\omega}{2} \left(n + \frac{1}{2} \right)$$